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14. ABSTRACT

Many contemporary problems in science ranging from the spread of hazardous chemical or nuclear plumes to protein folding in molecular dynamics to scale up of small scale effects in nanotechnology, to making accurate predictions of the coupled atmosphere-ocean system involve partial observations of extremely complicated systems with many degrees of freedom. There is a practical need to develop accurate real-time predictions of these extremely complex multi-scale dynamical systems with many degrees of freedom. Novel mathematical issues arise in the attempt to quantify the behavior of such complex multi-scale systems. New mathematical issues arise in the practical application of these filtering strategies to complex spatially extended systems in order to do rapid prediction including assessments of uncertainty from model error and parameter estimation and this is the focus for the present seed proposal.

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Final Report: Real Time Filtering and Parameter Estimation for Dynamical\ Systems with Many Degrees of Freedom
Award Number: **N00014-07-1-0750**

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Background:
Bayesian hierarchical modeling and reduced order filtering strategies have been developed with some success in these extremely complex systems. The basis for such dynamic prediction strategies for the complex spatially extended systems is the classical Kalman filtering algorithm.

Objective:
Many contemporary problems in science ranging from the spread of hazardous chemical or nuclear plumes to protein folding in molecular dynamics to scale up of small scale effects in nanotechnology, to making accurate predictions of the coupled atmosphere-ocean system involve partial observations of extremely complicated systems with many degrees of freedom. There is a practical need to develop accurate real-time predictions of these extremely complex multi-scale dynamical systems with many degrees of freedom. Novel mathematical issues arise in the attempt to quantify the behavior of such complex multi-scale systems. For example, in the coupled atmosphere-ocean system, the current practical models for prediction of both weather and climate involve general circulation models where the physical equations for these extremely complex flows are discretized in space and time and the effects of unresolved processes are parametrized according to various recipes; the result of this process involves a model for the prediction of weather and climate from partial observations of an extremely unstable, chaotic dynamical system with several billion degrees of freedom. New mathematical issues arise in the practical application of these filtering strategies to complex spatially extended systems in order to do rapid prediction including assessments of uncertainty from model error and parameter estimation and this is the focus for the present seed proposal.

Approach:
Novel Approaches to Issue #1 Practical Mathematical Criteria for Increasing Filter Ensemble Size: The PI has been developing a new mathematical theory to address the

possibilities for using such radical numerical strategies to increase ensemble size. One of the PI's reference contains the first elementary mathematical theory supporting this possibility and an explicit demonstration; utilizing this theory demonstrating stable accurate filtering (with a single ensemble member!) with a strongly unstable difference approximation to a stochastic advection-diffusion equation. The failure of standard observability criteria as guidelines is noted. The PI has developed a new mathematical theory, mimicking von Neumann stability analysis for difference equations, for stable accurate filtering with unstable/stable difference approximations to stochastic PDE's. Such a theory is not obvious since filtering algorithms are nonlinear and provides the hope to provide realistic offline test criteria as mathematical guidelines. It is shown how unstable difference approximations can nevertheless, result in a small mean model error as an application of the theory.

Novel Approaches to Issue #2 Information Flow in Complex Systems: The PI has been developing techniques utilizing information theory in a computationally feasible fashion in systems with many degrees of freedom and with large or small ensemble sizes in prediction; these techniques have been tested and validated on many degrees of freedom long-range forecast models for the atmosphere as well as toy models in several contexts. There are important challenges involving information flow between components of complex subsystems to quantify model error in filtering, prediction, and parameter estimation. The PI has two very recent books discussing applications of information theory for complex systems.

Novel Approaches to Issues #3: The PI and co PI have developed mathematical theories for stochastic mode reduction over many years and applied them to realistic dynamical core models for the atmosphere with thousands of degrees of freedom where statistically accurate reduced stochastic models involve roughly ten or less degree of freedom have been. The PI has developed novel methods for coarse-graining stochastic lattice models (Markov jump processes) coupled to large scale equations with an enormous increase in computational efficiency (factors of tens of thousands to a billion!). This is an active enterprise of the PI's which directly impacts these issues.

Novel Approaches to Issue #4: Numerical techniques for multiscale dynamical systems with stochastic effects. The co-PI has introduced new kind of numerical methods for multiscale dynamical systems with stochastic effects. These methods build on limit theorems for singularly perturbed Markov processes, originally developed in the 70s by Khasminskii, Kurtz, Papanicolaou, etc. Under suitable assumptions, these limit theorems provide one with closed effective equations for the slow variables in the system; the coefficients in these equations are given by expectations over the statistics of the fast variables conditional on the value of the slow variables. In general, these expectations cannot be computed analytically, but it is possible to estimate them on-the-fly when needed via short runs of the fast variables. Once this is done, the slow variables can be evolved using the effective equations by one macro-time-step, and the procedure can be repeated. Overall, the numerical cost of the algorithm is independent of the small parameter" $\varepsilon \ll 1$ measuring the separation of time scale between the fast variables in the system and the slow ones; in contrast, the cost of standard numerical schemes scales as $\varepsilon{-1}$. In a series of works the co-PI has shown that these new numerical procedures are effective in various contexts, including polymeric fluids. The co-PI has also shown that, in certain situations, these new numerical procedures can be made seamless in the sense they can be applied to systems in

which slow and fast variables exist but are not known explicitly. The only requirement thing is that it be possible to partition the velocity fields driving the system into fast and slow components. This is clearly a very suitable property as the identification of the slow and fast variables is often very difficult in realistic systems, whereas the amplitude of the driving field is usually readily accessible. We propose to pursue the developments of new techniques in this direction.

Accomplishments:
Mathematical guidelines to guarantee accurate statistical filtering in real time for complex dynamical systems with many degrees of freedom; Assessments of stochastic mode reduction and "on the fly" numerical procedures for complex multi-scale models. These results include model error, the role of ensemble size, parameter estimation, etc. Applications to complex prototype problems in atmospheric science, biological systems, material science, etc. demonstrating statistical filtering, etc.

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